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In this grant the electronic structure of rare earth pnictides (Erbium and Gadolinium arsenides, Phosphides and Nitrides) and related materials (Scandium nitride and arsenide) were investigated using first-principles calculations. The work provided theoretical support for a number of on-going experimental studies of the magnetotransport and interfacial properties of these materials and related devices. It identified new possible applications of these materials based on their magnetic properties.

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Rare Earth Compound Integration with Semiconductors

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Abstract

In this grant the electronic structure of rare earth pnictides (Erbium and Gadolinium arsenides, phosphides and nitrides) and related materials (Scandium nitride and arsenide) were investigated using first-principles calculations. The work provided theoretical suppport for a number of on-going experimental studies of the magnetotransport and interfacial properties of these materials and related devices. It identified new possible applications of these materials based on their magnetic properties.

to provide a fully quantitative account of the spin-dependent transmission coefficient within a model description.

In the third year of the project, we completed studies of the ErAs/GaAs Schottky barriers. This study addressed the extensive set of experimental data obtained by Palmstrøm et al. [6] on this system and is important for a full understanding of the integrated systems. This work was again performed in collaboration with Petukhov (at SDSMT). We started by doing extensive calculations of the (001) interface. Full-potential linear muffin tin orbital calculations were carried our to optimize the interface structure for two models suggested by experiment: the chain model and the shadow model. In the first, the GaAs is terminated in Ga, in the second it is terminated in As. One can alternatively think of the first model as resulting from a conversion of the top As layer of GaAs into the first ErAs layer. Subsequently, we analyzed their electronic structure by calculating partial densities of electronic states, charge densities, etc. These time consuming calculations finally led to the main conclusion that the interface bonding is weak. For example, for the chain model, the interface ErAs layer is found to debond from the GaAs resulting in a 60 % increase in the interplanar distance between Ga terminating layer and the first ErAs layer. The charge densities showed dangling bond character. Also, it was found that the Fermi level of the models was pinned by interface states resembling surface dangling bond states. Hence, we decided it would be useful to compare the interface PDOS with that of the surfaces of the individual components, in particular with the GaAs surfaces. These GaAs calculations were carried out for the same thin slab models as occuring in the ErAs/GaAs interface model. PDOS of both interface and surface were obtained using the atomic sphere approximation LMTO version but using the structure obtained from FP-LMTO. The comparison showed very clearly that the interface states are similar to the corresponding free surface states of our GaAs surface models. This constitutes an important insight which provides a simple way for speculating about the interfaces of other crystallographic orientation. This led to some first insights into the reason for the orientation dependence of the SBH. The results of this work were presented at the AFOSR program review in Santa Barbara in August 97 and submitted for pbulication in Solid State Communications.[7] They were also presented at the Fall MRS meeting and a paper on these results was accepted for the conference proceedings.[8]

Finally, as already mentioned, we returned to the question of the semiconducting or semimetallic nature of the nitrides in this family. Our initial work [3] had indicated that there would possibly be a very interesting semiconductor to semimetal transition in GdN induced by a magnetic field. The reason is that above the Curie temperature (about 40K in GdN) (and in the absence of a magnetic field), the Gd spins are randomly oriented, thus providing no net spin polarization in the bands in a mean field sense. In this case the LDA predicts the system to have a zero gap, but as noted above, a small indirect (Γ-X) gap can be expected due to corrections beyond LDA. In a magnetic field, one expects the local moments to align. The system is then described by the local spin density approximation. The spin splitting of the lowest conduction band would then lead to a gap closing if the spin-splitting is greater or equal to the initial (zero-field) gap. In addition, this system would then become a so-called half-magnetic system. This is a system in which there is a gap for one spin orientation and no gap for the other. This means that a perfect spin-filter could possibly be made from such a material. Needless to say, this prospect is quite interesting and was found worthy of further investigation.

Furthermore, another interesting effect had been predicted in the literature (in the 80's) for the closely related system ScN. In the case of an almost zero gap semimetal, it was predicted by Monnier et al. [9] that at low temperature, spontaneous exitation of electron-hole pairs could occur and lead to a lowering of the energy by condensation into a electron-hole correlated groundstate (similar to electron-hole droplets that can be produced in e.g. Ge by laser excitation at low temperature). The evidence for this in ScN, however, was (in our opinion) not entirely conclusive because Nitrogen vacancies might have led to a degenerate n-type semiconductor and no conclusive evidence of semimetallic behavior as opposed to degenerate n-type was presented. We further realized that in GdN, the spin-polarization effects would provide an opportunity to

3 Collaborations and Impact.

This work was performed in collaboration and close contact with several experimental groups working mostly on ErAs films and their properties and devices. These are the groups of S. Jim Allen, Jr. at the University of California at Santa Barbara, Chris Palmstrøm at the University of Minnesota in Minneapolis, whose initial work on these materials was done while at Bell Core and has been funded by AFOSR, and Ria Bogaerts and Fritz Herlach at the University of Leuven (in Belgium). Our work on the magnetotransport and the resonant tunneling was directly inspired by these collaborations. We also acknowledge very useful discussions with C. Palmstrøm on the Schottky barrier height problem.

C. Palmstrøm and B. Segall organized a focused session at the APS March Meeting in 1996 dedicated to rare earth and transition metal integration with semiconductors. This Focused session was quite successful and brought researchers on rare-earth compounds together with people from the dilute magnetic semiconductor community.

Last, but not least we maintained an active collaboration with Andrei Peukhov, who was a postdoctoral researcher on the project in the first year and later moved to the South Dakota School of Mining and Technology (SDSMT). His work at SDSMT was funded by AFOSR-Epscor.

4 Conclusions and Outlook

In conclusion, we have established basic electronic structure properties of the rare-earth pnictides (in particular the arsenides, phosphides, and nitrides of Gadolinium and Erbium) and used them to provide a solid understanding of the available experimental data on $Er_xSc_{1-x}As$ films and related devices such as magnetotransport measurements and resonant tunneling. We have also provided improved understanding of the ErAs/GaAs interface atomic and electronic structure. Our work has in addition identified interesting new properties which could lead to future applications of these materials. These generally are associated with the magnetic field tunability of the electronic structure due to the strong exchange coupling of RE localized moments with the valence and conduction states. We have mentioned already that this may lead to materials which are switchable from transparent to opaque by a magnetic field and possibly to spin-dependent diodes. We also anticipated strong magneto-optic Kerr rotation and Faraday rotation effects in this class of materials based on recent work of Pittini et al. on CeSb.[11] Finally, we have identified the nitrides of this family as an interesting class of relatively narrow-gap semiconductors with extremely interesting properties. These are further enhanced by the opportunity of combining this with sharp line intra 4f manifold optical excitations and the associated luminescence (in particular in Er^{3+}).

We thus anticipate that this class of materials may find interesting applications in optoelectronics when integrated with semiconductors and are worthy of further development. We plan to submit a future proposal to AFOSR to pursue these ideas.

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[2] A. G. Petukhov and W. R. L. Lambrecht, Electronic Structure of Rare-Earth Pnictides for Metallization of Semiconductors, in *Advanced Metallization for Devices and Circuits — Science, Technology and Manufacturability*, ed. by S. P. Marurka, K. N. Tu, A Katz, and K. Maex, Mater. Res. Soc. Symp. Proc. Vol. 337, (MRS, Pittsburgh 1994), p. 583-8

[3] A. G. Petukhov, W. R. L. Lambrecht, and B. Segall, Electronic structure of rare earth pnictides, *Phys. Rev. B*, **53**, 4324 (1996).

5.2 Invited talks

1. W. R. L. Lambrecht, Rare-earth pnictides, opportunities for physics and applications, Midwest Solid State Theory Symposium, Columbia, MO, Oct. 15-16, 1994
2. W. R. L. Lambrecht, Spin-polarization effects in rare-earth group-V compounds, APS March Meeting 1996, Focused Session on Rare Earth and Transition Metal Integration with Semiconductors

5.3 Other Presentations

1. A. G. Petukhov and W. R. L. Lambrecht, Electronic Structure of Rare-Earth Pnictides for Metallization of Semiconductors, MRS Spring Meeting 1994.
2. A. G. Petukhov, W. R. L. Lambrecht and B. Segall, Quantum confinement effects in ultrathin layers of Rare Earth Group-V compounds, MRS Fall Meeting, Boston, November 1994
3. A. G. Petukhov, W. R. L. Lambrecht and B. Segall, Quantization in rare-earth group-V/semiconductor superlattices, Bulletin Am. Phys. Soc. **40** (1995) 637 (N14.7) APS March Meeting 1995
4. A. G. Petukhov and W. R. L. Lambrecht, Schottky barriers heights at ErAs/GaAs interfaces, Materials Research Society Fall Meeting, Boston 1995, Symposium on Spectroscopy of Heterojunctions,
5. Andrey G. Petukhov, Brian Hemmelman, Walter R. L. Lambrecht, Schottky barrier formation at ErAs/GaAs (001) interfaces, Bull. Am. Phys. Soc. **42**, O17.12, p. 678 (1997).
6. A. G. Petukhov, W. R. L. Lambrecht and B. Segall, Electronic states in ErAs quantum wells, *Bull. Am. Phys. Soc* **41** (1996), p. 44, abstract A26.3 American Physcial Society March Meeting 1996,
7. AFOSR Review at UCSB, Aug. 18-20, 1997, W. R. L. Lambrecht, Theory of semimetallic rare-earth compound heteroepitaxial structures.
8. A. G. Petukhov, B. Hemmelman, and W. R. L. Lambrecht, Equilibrium structure and Schottky bariers at ErAs/GaAs interfaces, MRS Fall Meeting, 1997.